REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
06-07-2004

2. REPORT TYPE
Final Technical Report

3. DATES COVERED *(From - To)*
Oct 1998 - Sep 2003; Jul 2004

4. TITLE AND SUBTITLE
Assessing Transport in the Ocean and Atmosphere: Computational Tools for Predictability and Experimental Design

5a. CONTRACT NUMBER

5b. GRANT NUMBER
N00014-99-1-0029

5c. PROGRAM ELEMENT NUMBER

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

6. AUTHOR(S)
Miller, Patrick, D

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Stevens Institute of Technology
Castle Point on Hudson
Hoboken, NJ 07030

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Code 322MM, Ballston Tower One, Room 428
Office of Naval Research
800 North Quincy Street
Arlington, VA 22217-5660

10. SPONSOR/MONITOR'S ACRONYM(S)
ONR / OAS

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for Public Release; distribution is Unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT
This effort addressed applications of dynamical systems to aperiodic, two-dimensional velocity fields, and improvements in the numerical tools available to perform such analysis. Invariant manifold techniques were used to estimate the extent of mixing in a barotropic meandering jet (Gulf Stream), showing that transport is on the same order as cross-jet transport due to ring detachment. Manifold calculations verified theoretical predictions of separatrix splitting in a viscous perturbation of the barotropic pv equation. In a simulation of an island recirculation, lobe analysis shed light on the importance of chaotic transport relative to Ekman transport. A pv budget was calculated for the gyre using a Lagrangian definition of the recirculation. The results imply that the budget for a time-averaged fixed boundary may typically overestimate the importance of chaotic advection in the overall vorticity budget. The vftool software package went through a major rewrite, including a better ODE solver, improved command-line interface and model input, a greatly expanded and improved Matlab toolbox, and compatibility with several variants of Unix.

15. SUBJECT TERMS
dynamical systems, transport, mixing, chaotic advection, invariant manifolds, lobe analysis, barotropic vorticity equation, meandering jet, recirculation, eddy, gyre, scientific computing, computational science

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
				7	Patrick D. Miller

19b. TELEPHONE NUMBER *(Include area code)*
201-216-5452

Assessing Transport in the Ocean and Atmosphere: Computational Tools for Predictability and Experimental Design

Patrick D. Miller

Stevens Institute of Technology
Department of Mathematical Sciences
Castle Point on Hudson
Hoboken, NJ 07030
phone: (201) 216-5452 fax: (201) 216-8321 e-mail: pmiller@stevens.edu

Award Number: N00014-99-1-0029
Final Technical Report

OBJECTIVES

There has been significant interest in applying geometric techniques from dynamical systems to the study of transport and mixing in oceanic flows. Much of this has been based on the idea that stable and unstable manifolds of hyperbolic trajectories provide a useful geometric description of transport and mixing processes when the velocity fields are two-dimensional and periodic in time. Original objectives of this research effort included:

- applying these dynamical systems techniques to flows with aperiodic time-dependence
- identifying additional diagnostics relevant to transport that can be acquired from the invariant manifold template
- extending the functionality of the existing *vftool* numerical package and improving the computational efficiency and numerical accuracy of the algorithms
- making the computational tools more accessible to others including better interfaces for incorporating new models and integration with computational environments such as *Matlab*

The software is especially suited to analyze velocity fields that are given as data sets; velocity fields derived either as output from numerical simulations of the governing dynamical equations, or derived from observations in the real environment.

BACKGROUND

Within time-dependent, two-dimensional velocity fields, regions of strong saddle-type dynamics play a significant role in enhancing transport and mixing of fluid. When the time-dependence is periodic, asymptotic ($t \to \pm\infty$) structures such as stable and unstable manifolds of hyperbolic periodic trajectories provide a geometric template describing this transport and eventual mixing. In this case it is sufficient to analyze the dynamics of the two-dimensional Poincaré map, where the transport is described by the transverse intersections of one-dimensional stable and unstable manifolds associated with hyperbolic fixed points [5], [9].

When the velocity fields exist as data sets, the time-dependence is generally aperiodic, the fields are defined only on a finite interval in time, and a single two-dimensional map is no longer sufficient to describe the transport dynamics. This aperiodic time-dependence and finite-time aspect of numerical velocity fields motivated new computational techniques for identifying dynamical structures useful in characterizing transport and mixing. Methods developed with collaborators at Brown University and Woods Hole are used to define certain distinguished two-dimensional invariant manifolds which behave much like asymptotic stable and unstable manifolds on the available finite time interval [7], [3]. These *effective* invariant manifolds can be identified numerically by evolving an appropriate set of passive tracers (solutions to the ODE, $\mathbf{x}'(t) = \mathbf{v}(t, \mathbf{x})$). If the initial tracer positions straddle the hyperbolic region, the fluid particles trace the unstable manifold in forward time and the stable manifold when the ODE is run in reverse with respect to time. As the manifolds lengthen, the numerical algorithm must start additional tracers to keep the manifolds accurately resolved.

When viewed at a fixed time, the manifolds for two-dimensional vector fields appear as curves in the phase space. Segments of these manifolds can be used to define time-dependent boundaries (Lagrangian boundaries) between different regions of the flow. When the manifolds intersect, lobes are formed; closed regions in the phase space bounded by two segments of manifolds, one stable and the other unstable, connecting a pair of intersection points (hetero- or homoclinic trajectories). As these lobes evolve in time, they are associated with an exchange of fluid between the two regions, a mechanism often referred to as “chaotic advection” or “chaotic transport”. The area of the lobes formed from the intersection of these manifolds can be used to quantify the material transport across these boundaries [7].

RESULTS

Barotropic meandering jets

In work with Rogerson, Pratt, and Jones [10], stable and unstable manifolds were identified in simulations on a fully nonlinear, dynamically consistent, barotropic model of a meandering jet. The manifolds confirmed that the most significant exchange of fluid is between the eddies that bound the jet and the region outside the jet. Fluid exchange between the eddies and the jet itself was 4–7 times smaller, consistent with earlier results involving simpler kinematic models [6]. When dimensionalized to the scale of the Gulf Stream, the volume transport associated with this mechanism of "chaotic advection" was comparable to the fluid crossing the Gulf Stream due to the mechanism of ring detachment.

In a related result by Lozier et al [4], RAFOS float trajectories in the vicinity of the Gulf Stream were viewed in a moving frame. The fate of the trajectories were then interpreted based on the dynamical systems analysis from this numerical model of meandering jets.

Viscous perturbations of vorticity conserving flows and separatrix splitting

In joint work with Sandstede, Balasuriya, and Jones [11], these numerical techniques were used to identify stable and unstable manifolds in a time-dependent, two-dimensional velocity field that satisfies a viscous perturbation of the barotropic vorticity equation on the β-plane. This paper extended earlier results from Balarsuriya’s Ph.D. thesis [1] by developing a Melnikov theory applicable to vector fields defined over finite, but sufficiently large time intervals. In this model problem we had an exact solution to the perturbed barotropic equation. The numerical computations confirmed the predicted separatrix splitting and the non-existence of heteroclinic points (see Figure 1). The distance of the splitting as determined from the numerical simulations compared favorably with the theoretical values.

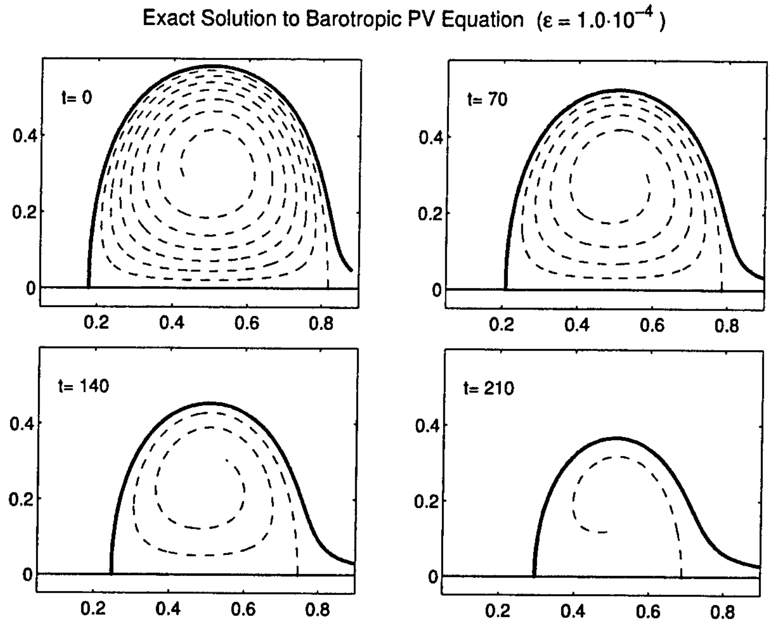

Figure 1. Computed manifolds for $\varepsilon = 1 \times 10^{-4}$*. The particle trajectories satisfy the equations,* $x'(t) = -\psi_y(x, y, t)$ *and* $y'(t) = \psi_x(x, y, t)$*, where the streamfunction* ψ *satisfies the partial differential equation,* $q_t - \psi_y q_x + \psi_x q_y = \varepsilon \Delta q$ *with potential vorticity* $q = \Delta\psi + \beta y$*.*

Chaotic transport for an island recirculation

In work with Pratt, Jones, and Helfrich [12], lobe analysis was used to analyze a time-dependent, boundary-trapped recirculation. The recirculation gyre occurs in a numerical model of wind-driven flow around an island, with a geometry similar to persistent eddies such as the Alboran Gyre and The Great Whirl. In the numerical model, an anti-cyclonic circulation is driven by a steady wind stress, setting up a large recirculation gyre to the east of the island. The forcing is parametrized as the ratio of the inertial boundary layer thickness, $\delta_I = (U/\beta)^{1/2}$, to the Munk boundary layer thickness, $\delta_M = (A_H/\beta)^{1/3}$. Here U denotes a horizontal velocity scale for the flow and A_H the horizontal eddy viscosity. Throughout the numerical experiments δ_M was held fixed at 40 km. For $\delta_I/\delta_M = 1.0$ the flow is steady and the only material transport between the gyre and the surrounding fluid is due to a downward "Ekman pumping", a volume flux that can be estimated from theory.

As δ_I/δ_M increases, the two-dimensional velocity field becomes time-dependent although the recirculation attached to the island boundary persists for long times providing an ideal coherent structure for studying Lagrangian transport. The effective stable and unstable manifolds emanate from hyperbolic regions close to the island boundary and at either end of the gyre. As the forcing is increased in these simulations, the lobe geometry becomes less regular in both time and space. Representative lobes are shown in Figure 2 for increasing values of δ_I/δ_M.

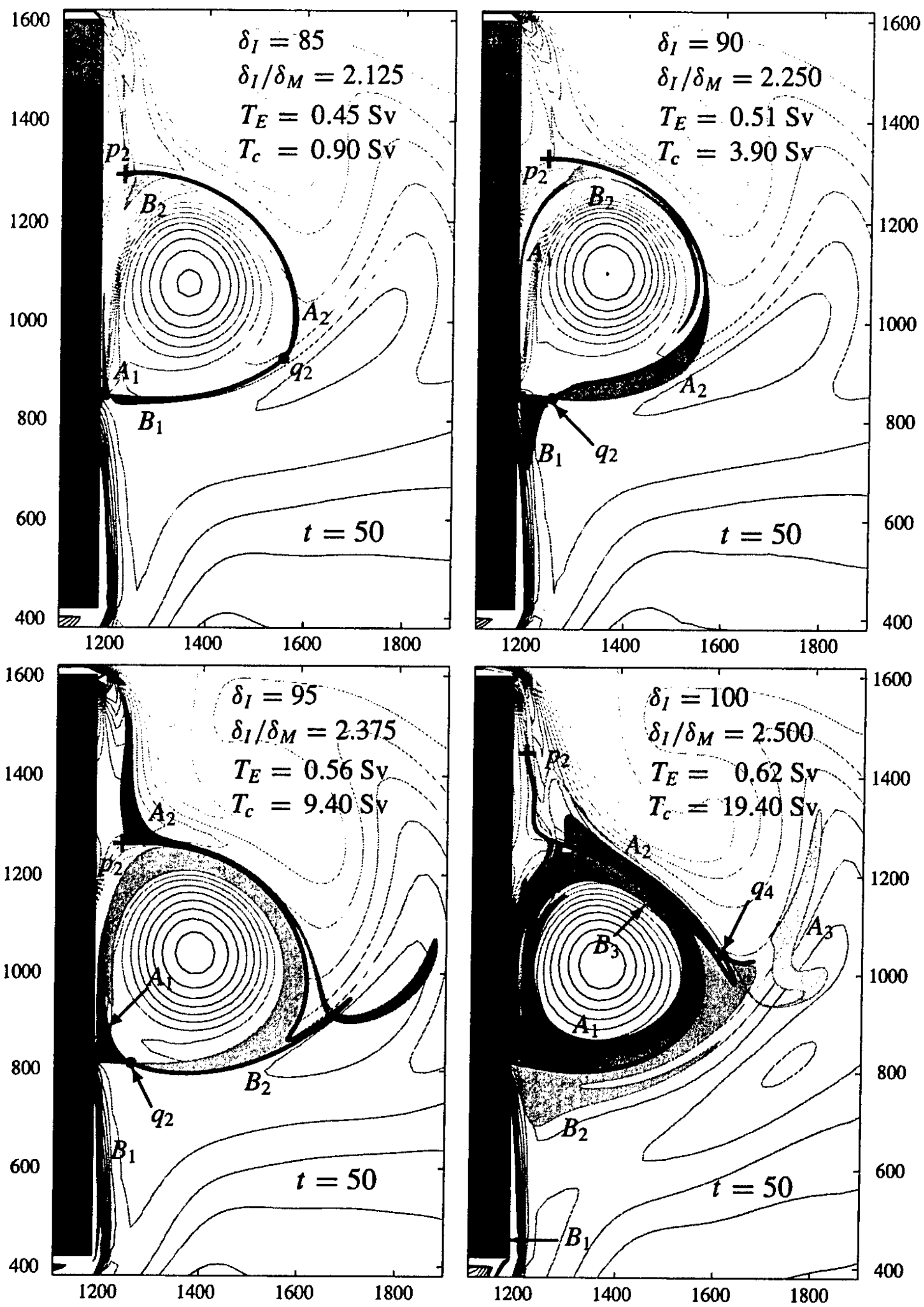

Figure 2. Lagrangian transport for the numerical simulations of flow past an island. The Munk layer thickness, δ_M, is fixed at 40 km in all four runs. The manifolds were evolved for 50 days. T_E denotes the Ekman transport and T_c the chaotic transport.

The analysis shows that the transport out of the gyre due to Ekman pumping (T_E) is quickly surpassed by transport fluxes associated with chaotic advection (T_c). Figure 3 is a graph comparing the Ekman transport to the transport due to chaotic advection. The Ekman transport is equal to the downwards Ekman pumping velocity integrated over the fixed area of the recirculation as determined by linear theory [8]. A least-squares fit yields the parametrization, $T_c \approx 0.54[(\delta_I/\delta_M)^2 - (1.8)^2]^{3.2}$. The shaded region in Figure 3 is an estimate of the range in δ_I/δ_M over which the method of lobe dynamics and the Lagrangian definition of the recirculation boundary is applicable and helpful.

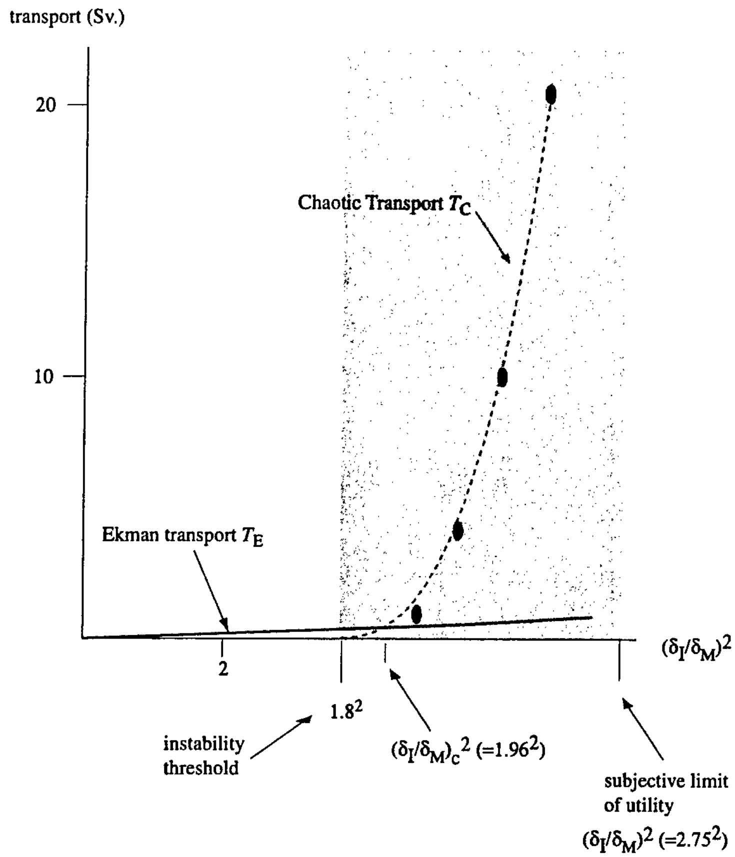

Figure 3. Ekman transport (solid line) vs. transport due to chaotic advection (dashed line). Note that T_E is independent of δ_M and is regarded here as a function of δ_I/δ_M only insofar as δ_M is fixed in the numerical experiments.

Potential vorticity budgets

As part of the analysis for the island recirculation we investigated methods for characterizing the potential vorticity budget of the recirculation gyre. We were interested in formulating approaches that consider the Lagrangian definition of the gyre as compared with a fixed recirculation boundary defined from the time-averaged velocity field. The most promising approach defines the Lagrangian boundary as segments of stable and unstable manifolds joined by a "gate". With this representation of the gyre, mass transport takes place through the gate continuously in time. The analysis showed that the fixed boundary from the time-averaged flow exaggerates the contribution from advection of vorticity into the gyre. This appears to be due in part to the recirculation passing as a whole across the fixed boundary, rather than a true vorticity flux at the boundary of the gyre.

Advances in software (vftool)

This effort included a number of significant improvements to the numerical tools used for performing the dynamical systems analysis.

- added adaptive-step method for solving the differential equations (Runge-Kutta-Fehlberg method)
- overhauled package of C-code to simplify the model inputs, improve the command-line interface, and add help files
- code now runs under irix, linux, netbsd operating systems
- overhauled Matlab toolboxes for performing data analysis, eliminated i/o problems due to system-dependent byte order for unformatted data, added complete help pages for all m-files

Several other programming features also received attention but had not reached the point of being fully implemented into the working code by the end of the funding period.

- solving the linearized variational equations along with the nonlinear differential equations; this will provide additional characterization along the lines of Haller's work [2]
- parallelizing the code to speed up manifold calculations which require tracking thousands of fluid particles
- representing the material curves using a C^1 interpolation; this includes tracking derivative information using the linearized flow and using error estimates to represent the curves more efficiently

PERSONNEL

In addition to the P.I., this program was supported by the efforts of one graduate student, Paul von Dohlen, and several undergraduate students, William Beksi, Shilpa Savaliya, Sunil Shah, and Wei Weng.

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